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**PROGRAM TO PRODUCE TABULATED DATA SET
DESCRIBING NSWC BURN MODEL FOR
HYDRODYNAMIC COMPUTATIONS**

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FOREWORD

The research effort documented in this report was performed under the Advanced Technology Torpedo Thrust Program and funded by Office of Naval Technology. A general purpose program has been developed which applies the concepts of the NSWC Burn Model and generates a tabulated data set. From this tabulated data set, any one-, two-, or three-dimensional hydrocode containing a reactive mixture scheme can determine a new burn fraction based on a previous burn fraction, pressure, and time step.

The illustrations in this report appear after the body of the report.

The author wishes to acknowledge the helpful insights of Dr. Raafat Guirguis of the Naval Surface Warfare Center on how the NSWC Burn Model works, and Drs. Schittke and Feisler of Industrieanlagen-Betriebsgesellschaft for their suggestion to develop a general purpose program to tabulate the data and an example of how to proceed with the effort.

Approved by:

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SECTION 1

INTRODUCTION

This report describes the transformation of the NSW Burn Model, described in Reference 1, into a general purpose program which produces a simple set of information. This information can be transformed into a tabular database that can be used by any one-, two-, or three-dimensional hydrocode which contains a reactive mixture scheme. The term, general purpose program, is used throughout this report to emphasize the fact that the computer program which produces the tabulated data set is separate from the hydrocode run which uses the tabulated data set.

The basic equations, described in Reference 1, which present the concepts of the NSW Burn Model are solved explicitly by a general purpose program in a Lagrangian coordinate system. These equations and the solution method are described in Section 2. Relationships which prescribe the necessary parameters for a hydrocode computation are shown in Section 3. Section 4 presents some conclusions and direction of future work.

SECTION 2

HOW THE NSWC BURN MODEL IS USED IN A GENERAL PURPOSE PROGRAM

The NSWC Burn Model assumes that a typical pore and binder in a high explosive can be modeled by a void region inside a sphere. Therefore, it is referred to as a hollow sphere model. The size of the hollow portion of the sphere representing the void and binder is in proportion with the global percentages of the component explosive, binder, and pore. The solid portion of the hollow sphere located between r_i , the minimum radius of the solid portion of the hollow sphere, and r_o , the maximum radius of the solid portion of the hollow sphere, is composed of the component explosive. Figure 1-a shows a typical situation in a real component explosive. Figure 1-b shows how the NSWC Burn Model views a typical situation in a real component explosive. Figure 1-c shows the region of computation of the NSWC Burn Model.

The NSWC Burn Model divides the portion of the sphere between r_i and r_o into a number of one-dimensional subcells which can be equally or geometrically spaced. In general, it seems that geometric spacing is more advantageous since the region requiring the greatest resolution is near r_i . This is due to the fact that the NSWC Burn Model is only used to determine the global burn fraction until a certain criteria is reached, indicating that surface burning has become predominant in determining the burn fraction. Then the global burn fraction can be determined according to a surface burn model.

It is assumed in the general purpose program presented here that the temperature throughout the hollow portion of the sphere representing the void and binder is constant. The value used for this region is equal to the value of the temperature at the location r_i initially, and at the location corresponding to the inner surface of the solid portion of the sphere as it moves into the solid region due to the conversion of solid subcells into burned gas products as time progresses. As time progresses, the small portion of burned gas products over all the subcells is collected in the hollow portion of the sphere in a cumulative manner.

In the general purpose program describing the NSWBC Burn Model, each subcell is bounded by two location values, the difference of which is the subcell width. The local burn fraction and temperature are found at the center of each subcell. The velocity is found at the two locations which bound the subcell region. Initially, it is assumed that the local burn fraction is zero, the temperature is the ambient temperature, and the velocity is zero for all subcells.

Initially, a pressure due to the surroundings, p_o , is applied at r_o and the pressure of the gas in the hollow portion, p_g , of the sphere is ambient pressure or some specified condition and applied at r_i . As the pressure, p_o , is applied to the outer surface of the hollow sphere model, it is assumed that there is a global mechanical deformation in progress near the pore, and that the material behavior is such that the stress is dependent on strain and strain rate. This results in an increase in p_g . The processes which occur are described in greater detail in Reference 1. Two assumptions are made, the elastic portion of mechanical deformation can be ignored and the bulk compressibility of the component explosive can be neglected. This greatly simplifies the equations needed to describe the NSWBC Burn Model for a hollow sphere.

Also, the location of the subcells in the hollow sphere model moves toward the center of the sphere as the pressure, p_o , is applied to the outer surface of the hollow sphere model. Likewise, as the component explosive begins to burn, the gas pressure, p_g , in the hollow portion of the sphere begins to increase, resulting in a force being applied to the surface located at r_i and directed toward the outer surface of the sphere. This results in additional changes to subcell boundary locations. The equation used to determine the velocity, $v(r,x,t)$, of the boundaries associated with each subcell is the following,¹

$$v(r,x,t) = \frac{\gamma (p_o - p_g - 2\sqrt{3} k \ln(r_o/r_i))}{2 (r_o^{-3} - r_i^{-3}) r^2 k} . \quad (1)$$

The variables used in Equation (1) are described below.

The basic equations used in the general purpose program to describe a hollow sphere model representative of the NSWC Burn Model in which an Arrhenius reaction is applied to the hot spot temperature which is modified by thermal diffusion, are the following,¹

$$\frac{d\lambda(x,t)}{dt} = \int_{r_i}^{r_o} \frac{\frac{d\Lambda(r,x,t)}{dt} 4 \pi r^2}{\frac{4}{3} \pi (r_o^3 - r_i^3)} dr , \quad (2)$$

$$\frac{d\Lambda(r,x,t)}{dt} = (1 - \Lambda(r,x,t)) Z \exp\left(-\frac{T^*}{T(r,x,t)}\right) , \quad (3)$$

$$T(r,x,t) = T_o(r,x,t) + \int_0^t \frac{dT}{dt}(r,x,t) dt , \text{ and} \quad (4)$$

$$\frac{dT(r,x,t)}{dt} = \frac{2.25 \gamma (p_o - p_g - 2\sqrt{3} k \ln(r_o/r_i))^2}{\rho C_p (r_i^{-3} - r_o^{-3}) r^6 k} + \frac{1}{\rho C_p} \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 k^* \frac{\partial T(r,x,t)}{\partial r} \right) + \frac{Q}{C_p} \frac{d\Lambda(r,x,t)}{dt}, \quad (5)$$

where r is the location of the subcell being evaluated at time, t ; $\lambda(x,t)$ is the global burn fraction of the system; $\Lambda(r,x,t)$ is the local burn fraction of an individual subcell in the hollow sphere model; and $T(r,x,t)$ is the temperature of an individual subcell in the hollow sphere model. Equations (3) through (5) are solved explicitly in the Lagrangian subcell coordinate system. The variable x indicates the global computational cell for which the hollow sphere model is being computed. For example, in a three-dimensional Cartesian coordinate system, x would be a function describing a unique X , Y , and Z location for the global computational cell. In the general purpose program described in this paper, the hollow sphere model is evaluated for one computational cell. Therefore, x is set to 1. $T_0(r,x,t)$ is the initial temperature of an individual subcell in the hollow sphere model, Z is the pre-exponential factor in the Arrhenius kinetics, T^* is the activation temperature, ρ is the density, k^* is the thermal conductivity, C_p is the heat capacity, Q is the heat of reaction of the explosive, and γ is a number which affects how fast the global burn fraction rises but not the asymptote to which the global burn fraction approaches. The values for the constants used to model PBX-9404¹ are shown in Table 1 on the next page.

Due to the nature of Equation (4) for $dT(r,x,t)/dt$, it is necessary to determine the quantity,

$$\frac{1}{\rho C_p} \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 k^* \frac{\partial T(r,x,t)}{\partial r} \right), \quad (6)$$

TABLE 1. PBX-9404 PARAMETERS USED IN THE NSW BURN MODEL

Z	5.0×10^{13}	μsec^{-1}
T*	26500	$^{\circ}\text{K}$
T ₀	300	$^{\circ}\text{K}$
ρ	1.84	g/cm^3
C _p	1.4×10^{-5}	$\text{cm}^2/\mu\text{sec}^2/^{\circ}\text{K}$
k	8.0×10^{-5}	Mbar
Q	5.439×10^{-2}	$\text{cm}^2/\mu\text{sec}^2$
k*	8×10^{-14}	$\text{cm}/\mu\text{sec}/^{\circ}\text{K}$
r _i	0.0039	cm
r _o	0.01	cm

for both boundaries of a subcell. This takes into account both the temperature transferred from the neighboring subcell on one side of a particular subcell and the temperature transferred to the neighboring subcell on the other side of a particular subcell.

The general purpose program which uses Equations (1) through (6) is shown in Appendix A. When running this program, the user is required to enter the time step for which the equations will be solved explicitly and the initial pressure, p_0 , applied to the hollow sphere. The user may specify, in the form of data statements in the general purpose program, the number of subcells in the component explosive portion of the sphere and, if geometric cell size expansion is used, the initial cell size and expansion factor from one cell to the next. The parameters shown in Table 1 are included in the form of data statements in the general purpose program.

The general purpose program iterates twice through the section which determines $d\lambda(x,t)/dt$, $d\Lambda(r,x,t)/dt$, $T(r,x,t)$, and $dT(r,x,t)/dt$ to converge to the solution. Iterations greater than two do not add significant improvements in convergence. The pressure of the gas is determined by using a JWL (Jones-Wilkins-Lee) Equation of State to model the component explosive gas products. The JWL Equation of State has the following form,

$$p = A \left(1 - \frac{\omega}{R_1 V}\right) \exp(-R_1 V) + B \left(1 - \frac{\omega}{R_2 V}\right) \exp(-R_2 V) + \frac{\omega}{V} E \quad (7)$$

where V , the relative volume, equals v/v_0 or ρ_0/ρ . The values for the JWL Equation of State parameters used to model PBX-9404² are shown in Table 2.

TABLE 2. JWL EQUATION OF STATE PARAMETERS USED FOR PBX-9404

ρ	1.84	g/cm^3
P_{CJ}	0.37	Mbar
D	0.88	$\text{cm}/\mu\text{sec}$
E_c	0.102	Mbar-cc/cc
R_1	4.6	
R_2	1.3	
ω	0.38	
A	8.524	Mbar
B	0.1802	Mbar
C	0.0121	Mbar

The relative volume, V , is found by the following method. First one multiplies the volume between r_i and r_e by the global burn fraction. This results in a quantity, v_0 , which takes into account the relative volume of the high explosive gas products from the component explosive. If v_0 is less than 1.E-11, it is set equal to 1.E-11. The current

volume of the hollow sphere, v_{hs} , and the volume of the binder, v_b , are also included in the determination of the relative volume which is given by the following expression,

$$V = \frac{v_{hs} + v_g - v_b}{v_g} . \quad (8)$$

Initially, it was desirable to create a model with constants that were solely determined by the physical parameters of the component explosive. However, the use of the JWL Equation of State to model the component explosive gas products introduces another set of unknowns which are usually determined through experiments such as cylinder tests or similitude data. In future applications of the general purpose program for high explosives that do not have JWL Equation of State parameters, it will be assumed that a generic set of JWL Equation of State parameters will be sufficient to model the gas products.

SECTION 3

HOW TO APPLY THE GENERAL PURPOSE PROGRAM RESULTS TO A HYDRODYNAMIC COMPUTATION

The general purpose program developed in the previous section for the NSWC Burn Model was designed to evaluate one hot spot formation caused by a constant pressure applied at the outer surface of the hollow sphere for the duration of the run. In a one-, two-, or three-dimensional hydrodynamic computation, there are many cells; each cell experiences varying pressure levels throughout the computation. In this section, a scheme for using the results of the general purpose program describing the NSWC Burn Model will be presented.

The first characteristic which needs to be defined is the transition from exponential growth of the reaction due to mechanical deformation to a slower growth of the reaction due to surface burning. This exponential growth of the reaction due to mechanical deformation can be thought of as the ignition phase of a hot spot. The equations and general purpose program presented in Section 2 describe this phenomena. The growth phase in which a transition to surface burning occurs is described with a different, simpler expression for the global burn fraction, such as a surface burn model. This expression is described in more detail in Reference 1.

After evaluating how different system parameters changed as the growth of the reaction slowed, it was observed that the quantity,

$$\log_{10} \left(\frac{\lambda(x,t) * \sum_{j=1}^n T(j,x,t) * dr(j,x,t)}{n * (r_o - r_i) p_o} \right), \quad (9)$$

changed sign, from a negative to a positive value, when the exponential growth of the reaction due to mechanical deformation slowed for every applied pressure (from 5 to 200 kilobar). The quantity represented by Equation (9) is independent of the time step selected. In Equation (9), $\lambda(x,t)$ is the global burn fraction, $T(j,x,t)$ is the temperature in the subcell, n is the number of subcells describing the component explosive, $dr(j,x,t)$ is the width of the subcell, r_o and r_i are the current values of the solid portion of the sphere which bound the component explosive region in the model, and p_o is the applied pressure as described in the previous section. When the quantity represented by Equation (9) changed sign in the general purpose program, it was assumed that the global burn fraction reached the transition point, λ_{hs} , at time, t_{hs} , where surface burning becomes the predominant mechanism.

When running a one-, two-, or three-dimensional hydrodynamic computation, another criteria, based on the computation, is used to determine when the transition from ignition to growth should be made. This transition to growth is based upon a minimum burn rate computed from both the ignition model and the growth model. This method of determining transition (presented above) provides enough information to reach and go slightly beyond the criteria of a hydrodynamic computation.

Important consideration also needs to be given when determining the minimum pressure below which a burn fraction will not accumulate in hydrodynamic computations. The general purpose program was run starting at a pressure of

200 kilobar. In each successive run, the pressure was reduced by 1 kilobar. It was determined that 5 kilobars is the lowest pressure that produced a smooth transition of λ_{hs} from one pressure to the next. At 6 kilobars, the value of λ_{hs} was $4.92e-3$; at 5 kilobars, the value of λ_{hs} was $4.15e-3$; and at 4 kilobars, the value of λ_{hs} was $1.22e-8$. Therefore, the lowest acceptable pressure has been selected as 5 kilobars. The data generated at 1 kilobar intervals includes the global burn fraction at transition, λ_{hs} , and the associated time at which this occurs, t_{hs} for each pressure.

For pressures of 5 kilobars, pressures of 10 to 100 kilobars at 10-kilobar intervals, and pressures of 100 to 200 kilobars at 20-kilobar intervals, the burn fraction versus time data is written out for every time step. This produced a large amount of data which was reduced to be easily handled by a hydrodynamic computation. The program which reduces the data, SLIM, is shown in Appendix B. In addition to data reduction, SLIM also normalizes the data, determines the length of the line resulting from the normalized data points, and determines the coordinates of points which divide the normalized line up into 400 equally spaced segments based on the original normalized data points. This allows the hydrodynamic computation to interpolate between two ranges of pressure to generate a normalized burn fraction versus time curve for any pressure. It also can be used to find the new burn fraction.

After much investigation, the following normalization scheme was found,

$$\log_{10} \left(\left(\frac{X}{X_{H.S.}} \right)^{\frac{P_{cc} Y}{P}} \right), \quad (10)$$

where Y is 0.15 when X is the time, Y is 0.05 when X is the burn fraction, P is the pressure in the cell, and P_{cc} is

the Chapman-Jouguet pressure of the high explosive. This normalization scheme seemed to work fairly well in creating curves from which one could interpolate. The normalized curves for 5 kilobars, 10 through 100 kilobars at 10-kilobar intervals, and 100 through 200 kilobars at 20-kilobar intervals are shown in Figure 2.

In order to use this information in a hydrodynamic computation, one tabulates the normalized curves in the form of data statements so that a hydrodynamic computation can determine the required information. The two programs, MAKEHS and MAKELAM, used to create the necessary data statements are shown in Appendix C. A sample subroutine which uses this information is shown in Appendix D. Currently, this subroutine is used in the Eulerian hydrocode DYSMAS.

The first time a cell experiences a pressure greater than a predetermined minimum, such as 5 kilobars for the case of PBX-9404, the value of the normalized time is determined using the time step as t , the current pressure in the cell as p_o , t_{hs} based on current p_o , and the Chapman-Jouguet pressure of the component explosive. From this, the associated burn fraction and burn rate can be determined. On subsequent cycles, the previous burn fraction is used to determine an old normalized time based on the current value of p_o . Then the current time step is used to determine a new normalized time and associated burn fraction and burn rate. Using this method, it is quite feasible to model the ignition phase with the NSWC Burn Model in conjunction with a simple surface burn growth phase model, and to run one-, two-, or three-dimensional hydrodynamic computations.

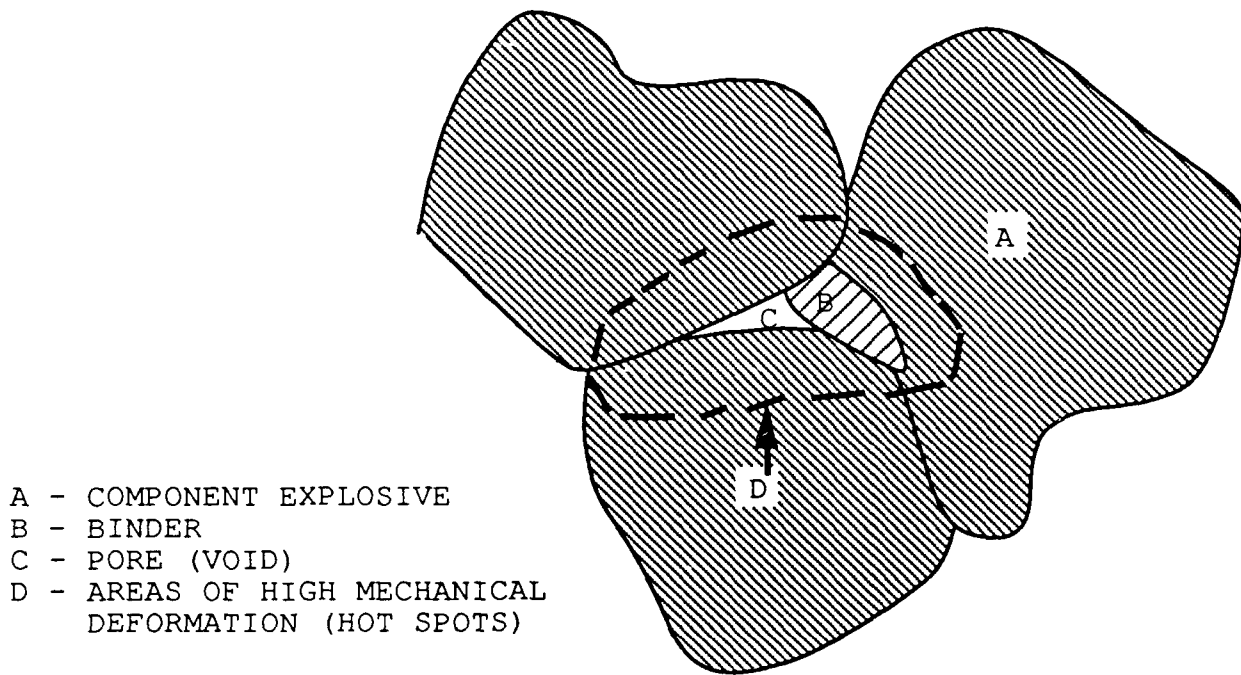
SECTION 4

CONCLUSIONS AND FUTURE WORK

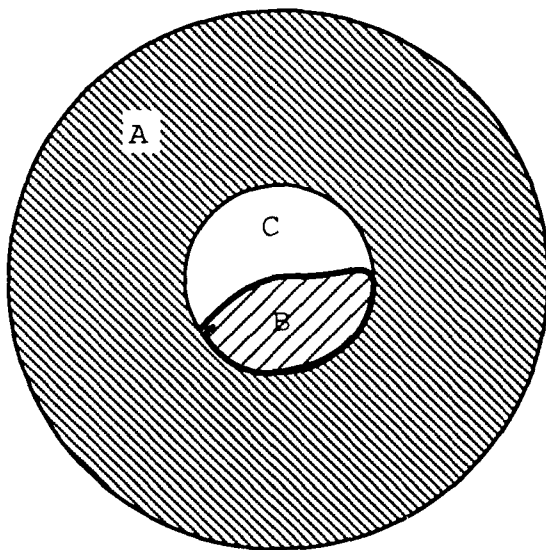
The development of a general purpose program to incorporate the concepts of the NSW Burn Model into a tabular data set have been successful. Future work will involve comparing results from inclusion of the tabulated data set into various hydrocodes to results shown in Reference 1. To complete this work, constants in the surface burn model may need to be modified to match the results shown in Reference 1.

Future work also will involve (1) verifying the assumption (discussed in Section 2) that a generic JWL Equation of State is sufficient because the parameters of the NSW Burn Model will compensate as needed, and (2) investigating whether the criteria for transition from ignition to growth phase will always be the quantity, shown in Equation (9), changing sign for different explosive components and/or similar explosive components with varying particle sizes, initial porosities, initial temperatures, and/or initial mass distributions between the component explosive and binder.

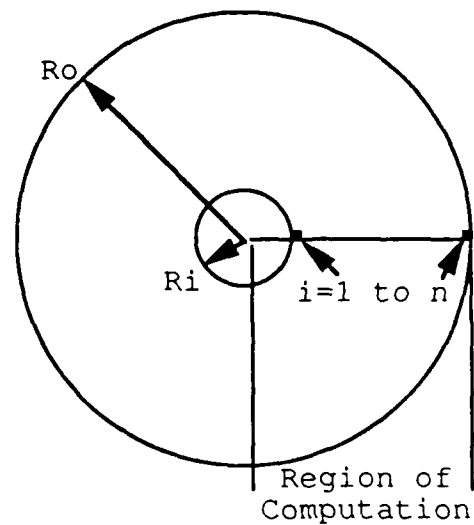
Planned improvements to the general purpose program include (1) implementing a numerical expression for the bulk compressibility of the binder to take into account the energy loss of compressing the binder, and (2) investigating a method of including shear-induced hot spot temperature effects.



(a) real situation in composite explosive

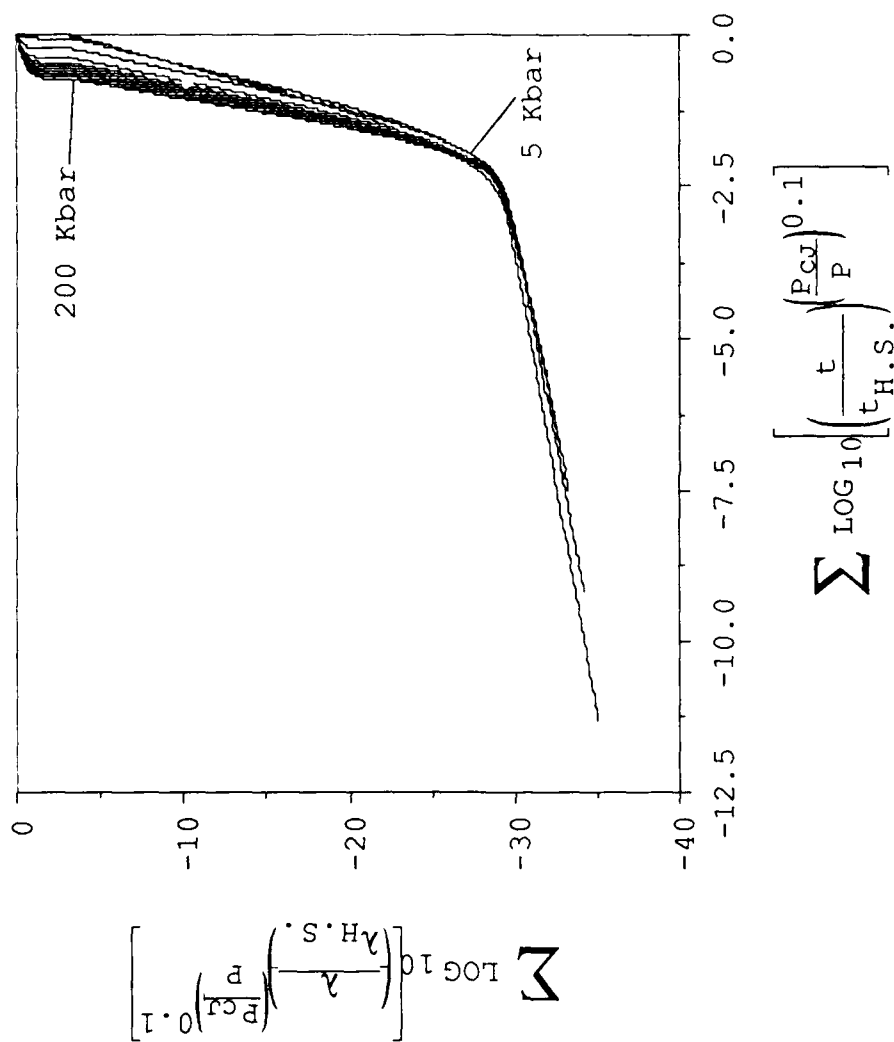


(b) one-dimensional approach of the NSWC Burn Model



(c) schematic of one-dimensional computational region of the NSWC Burn Model

FIGURE 1. THE NSWC BURN MODEL



NOTE: LINES CORRESPONDING TO INITIAL PRESSURES OF 10, 20, 30, 40, 50, 60, 70, 80, 90, 100, 120, 140, 160, AND 180 KILOBARS BOUNDED BY THE LINES CORRESPONDING TO 5 AND 200 KILOBARS

FIGURE 2. NORMALIZED DATA AT PRESSURES OF 5, 10, 20, 30, 40, 50, 60, 70, 80, 90, 100, 120, 140, 160, 180, AND 200 KILOBARS FOR PBX-9404

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2. Dobratz, B. M. and Crawford, P. C., LLNL Explosives Handbook: Properties of Chemical Explosives and Explosive Simulants, UCRL-52997, 31 Jan 1985.

APPENDIX A

GENERAL PURPOSE PROGRAM WHICH
IMPLEMENTS THE CONCEPTS OF THE NSWC BURN MODEL

```
c 3/4/91 version
  program test
    implicit double precision(a-h,o-z)
    dimension temp(450),clam(450),drrl3(450),rm(450),
1   tburn(450),dslmax(450),tempold(450),rmold(450)
    dimension rbd(451),rbd3(451),dr(450)
    data m/415/,factin/1.01/,cellin/0.000001/
    data z/5.e13/, tstar/2.65e4/, tambi/300./, rho/1.84/
    data cp/1.4e-5/, bulk/8.e-5/, q/5.439e-2/, stark/8.e-14/
    data ri/0.0039/, ro/0.01/, thrd/0.33333333/
    data ajwl/8.524011/, bjwl/0.1801812/, cmjwl/0.38/
    data rljwl/4.6/, r2jwl/1.3/, cjwl/0.012066373/
    write(6,*) 'input time step'
    read(5,*) dto
    compold=10000.
    totlen=ro-ri
    gam=0.025
    po=25.e-3
    type *, 'Enter initial pressure'
    read(*,*)po
    ms=1+(m-1)/10
    mpl=m+1
    nc=0
    tt=0.
c hot spots will not form if it takes longer than 1 microseconds
    t1=1.
    dt=dto
    ib=1
    istr=1
    rg=ri
    rg3=rg*rg*rg
    rbd(1)=ri
    rbd3(1)=rbd(1)**3
    ro3=ro**3
    ri3=rbd3(1)
    ro3mri3=ro3-ri3
    fako=2.25*gam/(rho*cp*bulk*(1./ri3-1./ro3)**2)
    fakr=3./(ro3mri3)
    fakp=po-3.464102*bulk*dlog(ro/ri)
    fakq=q/cp
    faks=1./cp/rho
    fakv=gam/2./bulk
    prev = cellin/factin
```

```

sum = ri
do i=1,m
  ipl=i+1
  prev=factin*prev
  dr(i)=prev
  if (sum+prev.lt.ro) sum=sum+prev
  if (i.eq.m) dr(i)=ro-sum
  temp(i)=tambi
  tempold(i)=tambi
  clam(i)=1.e-30
  tburn(i)=0.
  dslmax(i)=0.
  rbd(ipl)=dr(i)+rbd(i)
  rbd3(ipl)=rbd(ipl)**3
  drrl3(i)=rbd3(ipl)-rbd3(i)
  rm(i)=rbd(ipl)-0.5*dr(i)
  rmold(i)=rm(i)
end do
10 continue

c
c   determine volume of gas if not first time through
c
vo=slam*(rbd3(mpl)-rbd3(1))
if (vo.lt.1.d-11) vo=1.d-11
vbold=vb
vb=0.01*rbd3(mpl)
spvolg=(rbd3(1)+vo-vb)/vo
pgold=pg
pg=ajwl*dexp(-r1jwl*spvolg)+bjwl*dexp(-r2jwl*spvolg)+
1  cjwl*spvolg**(-omjwl-1)
if (istr.eq.1) pgbaseline=pg
if (istr.eq.1) pg=1.01323e-6
if (istr.ne.1) pg=pg+1.01323e-6-pgbaseline

c
c   determine new radial positions based on velocity
c
if (istr.ne.1) then
  riold=rbd(1)
  roold=rbd(mpl)
  do i=1,mpl
    v=fakv*(fakp-pg)/(1/ro3-1/ri3)/rbd(i)**2
    rbd(i)=rbd(i)+v*dt
    rbd3(i)=rbd(i)**3
  end do
  ro=rbd(mpl)
  ri=rbd(1)
  totlen=ro-ri
  ro3=rbd3(mpl)
  ri3=rbd3(1)
  ro3mri3=ro3-ri3
  do i=1,m
    dr(i)=rbd(i+1)-rbd(i)
    rm(i)=rbd(i)+dr(i)/2.
  end do
  fakp=po-3.464102*bulk*dlog(ro/ri)
  fako=2.25*qam/(rho*cp*bulk*(1./ri3-1./ro3)**2)
  fakr=3./(ro3mri3)

```

```

endif
tt=tt+dt
dslam=0.0
tempave=0.0
dtempave=0.0
do i=1,m
  if(clam(i).eq.1.d0)goto 55
  r=rm(i)
  r2dr=r*r*dr(i)
  clamold=clam(i)
  dslamold=dslam
  if(i.ne.1.and.i.ne.m)then
    deltemp=(tempold(i+1)-tempold(i))/(rmold(i+1)-rmold(i))
    deltempl=(tempold(i)-tempold(i-1))/(rmold(i)-rmold(i-1))
  elseif(i.eq.1)then
    deltemp=(tempold(i+1)-tempold(i))/(rmold(i+1)-rmold(i))
    deltempl=0.0
  elseif(i.eq.m)then
    deltemp=0.0
    deltempl=(tempold(i)-tempold(i-1))/(rmold(i)-rmold(i-1))
  endif
  subdtemp=deltemp*((rm(i+1)+rm(i))/2.0)**2
  subdtempl=deltempl*((rm(i)+rm(i-1))/2.0)**2
  subdtemp=faks*stark*(subdtemp-subdtempl)/r2dr
  do 54 jj=1,2
    tdt=tstar/temp(i)
    if(tdt.gt.100.0)type *, 'tstar/temp(i)',tdt
    if(tdt.gt.100.0)tdt=100.0
    dclam=(1.-clam(i))*z*dexp(-tstar/temp(i))
    dtemp=fako*(fakp-pg)**2/r**6+fakq*dclam+subdtemp
    clam(i)=dmin1(1.d0,clamold+dclam*tdt)
    if(clam(i).eq.1.d0)then
      dclam=(1.-clamold)/tdt
      dtemp=fako*(fakp-pg)**2/r**6+fakq*dclam+subdtemp+subdtempl
    endif
    temp(i)=tempold(i)+dtemp*tdt
    dslam=dslamold+fakr*dclam*r2dr
    if(clam(i).eq.1.d0)goto 55
54    continue
55    continue
  tempave=tempave+temp(i)*dr(i)
  dtempave=dtempave+dtemp*dr(i)
end do
istr=0
slam=slam+dslam*dt
do 56 i=1,m
  tempold(i)=temp(i)
  rmold(i)=rm(i)
56  continue
  rg3=rbd3(ib)+clam(ib)*drr13(ib)
  rg=rg3**thrd
  if(clam(ib).ge.0.999999d0) then
    tburn(ib)=tt
    dslmax(ib)=dslam
    ib=ib+1
  end if
nc=mod(nc+1,10)

```

```

mss=5
mdum=25
comp=tempave/m/totlen*slam/po
if(comp.eq.0.)comp=compold-1.
comp=dlog10(comp)
c hot spot lambda is reached according to criteria on next line
  if(comp.gt.0.0)goto 35
  compold=comp
  slamold=slam
  if(po.eq.0.01.or.po.eq.0.02.or.po.eq.0.03.or.po.eq.0.04
1   .or.po.eq.0.05.or.po.eq.0.06.or.po.eq.0.07
2   .or.po.eq.0.08.or.po.eq.0.09.or.po.eq.0.10
3   .or.po.eq.0.11.or.po.eq.0.12.or.po.eq.0.13
4   .or.po.eq.0.14.or.po.eq.0.15.or.po.eq.0.005)
1  write(8,'(1x,1p,5e13.5)')slam,dslam,comp,tt,pg
  if(tt.lt.tl.and.clam(m).lt.1.) goto 10
c the next line is designed to crash the batch job when t hot spot
greater than
c 1 microsecond.
  if(tt.ge.tl)acrash=1./0.
35  continue
  open(22,file='hs.info',status='unknown')
  do 838 ids=1,10000
    read(22,*,end=839,err=839)a,b,c
838  continue
839  continue
  write(22,'(7(1x,e15.7))')
1   po,tt-dt,slamold,pgold,riold,roold,vbold
  close(22)
  type *, 't hot spot = ',tt-dt,' slam = ',slamold
  stop
end

```


APPENDIX B

PROGRAM TO REDUCE AND NORMALIZE
OUTPUT FROM THE GENERAL PURPOSE PROGRAM

```

c compile with for/g_float
  implicit double precision(a-h,o-z)
  dimension asave(1000),dsave(1000)
  character*14 afile
  character*10 bfile
  aold=1000000.
  type *, 'enter file name to read'
  read(*,100) afile
100  format(a14)
     bfile(1:1)=afile(1:1)
     bfile(2:10)=afile(6:14)
     open(82,file=afile,status='old')
     open(84,file=bfile,status='new')
     inum=0
     do 120 i=1,1000000
       read(82,*,end=999) a,b,c,d,e
       anew=dlog10(a)
       if (dabs(anew-aold).gt..1.or.
1      (a.gt.0.0001.and.dabs(anew-aold).gt..01)) then
         inum=inum+1
         if (inum.gt.1000) stop
         asave(inum)=a
         dsave(inum)=d
         ipr=1
         aold=anew
       else
         ipr=0
       endif
120   continue
999   continue
     if (ipr.eq.0) then
       inum=inum+1
       if (inum.gt.1000) stop
       asave(inum)=a
       dsave(inum)=d
     endif
     type *, 'what is pressure,pcj'
     read(*,*) pres,pcj
     quanx=(pcj/pres)**.15
     quany=(pcj/pres)**.05
c convert to scaled quantities
  do 200 iic=1,inum
    asave(iic)=dlog10((asave(iic)/asave(inum))**quany)

```

```

        dsave(iic)=dlog10((dsave(iic)/dsave(inum))**quarx)
200    continue
c    find total length
        inumml=inum-1
        sumlen=0.
        do 210 iic=1,inumml
            sumlen=sumlen+dsqrt((asave(iic+1)-asave(iic))**2+
1            (dsave(iic+1)-dsave(iic))**2)
210    continue
        icar=2
        icarml=icar-1
        dellen=sumlen/400.
        curlen=0.0
        ruflen=0.0
        iflr=1
        write(84,431)dsave(1),asave(1)
        do 220 i=1,399
            curlen=curlen+dellen
230            if(iflr.eq.1)ruflen=ruflen+
1                dsqrt((asave(icar)-asave(icarml))**2+
2                (dsave(icar)-dsave(icarml))**2)
            if(curlen.gt.ruflen)then
                icarml=icar
                icar=icar+1
                iflr=1
                goto 230
            endif
            iflr=0
            dbtp=dsqrt((asave(icar)-asave(icarml))**2+
2            (dsave(icar)-dsave(icarml))**2)
            ari=dbtp-(ruflen-curlen)
            aval=ari*(asave(icar)-asave(icarml))/dbtp+asave(icarml)
            dval=ari*(dsave(icar)-dsave(icarml))/dbtp+dsave(icarml)
            write(84,431)dval,aval
220    continue
431    format(1x,f11.7,4x,f11.7)
        write(84,431)dsave(inum),asave(inum)
        stop
        end

```

APPENDIX C

PROGRAMS TO CREATE FORTRAN DATA
 STATEMENTS FROM THE TABULATED DATA SET
 FOR INCLUSION INTO A SUBROUTINE CALLED BY
 ANY ONE-, TWO-, OR THREE-DIMENSIONAL HYDROCODE

```

program makehs
parameter iam=500
dimension po(iam),ths(iam),alamhs(iam),pg(iam),ri(iam),
1      ro(iam),vb(iam)
open(81,file='hs.info',status='old')
icou=0
do 100 i=1,1000
read(81,*,end=999)po(i),ths(i),alamhs(i),pg(i),ri(i),
1      ro(i),vb(i)
icou=icou+1
100  continue
999  continue
open(82,file='hsdata.for',status='new')
write(82,110)icou,icou,icou,icou,icou
110  format(6x,'dimension po(',i3,'),ri(',i3,'),ro(',i3,
1      '),',/,5x,'1  alamhs(',i3,'),ths(',i3,')')
write(82,115)icou
115  format(6x,'data nrs/',i3,'/')
do 200 i=1,icou
write(82,120)i,ri(i),i,ro(i),i,po(i)
120  format(6x,'data ri(',i3,')/',e13.7,
1      '/',ro(',i3,')/',e13.7,'/',po(',i3,')/',f5.3,'/')
200  continue
do 210 i=1,icou
write(82,130)i,alamhs(i),i,ths(i)
130  format(6x,'data alamhs(',i3,')/',e13.7,'/', ths(',i3,')/',
1      e13.7,'/')
210  continue
stop
end

```

```

program makelam
implicit double precision (a-h,o-z)
character*10 filename
parameter iam=1000
dimension adum(iam),tdum(iam)
numfil=16
pcj=.370
filename(1:2)='f8'
filename(7:10)='.dat'
open(82,file='lamfile.for',status='new')
do 90 iiu=1,numfil
  if(iiu.eq.12)isep=iiu
  if(iiu.gt.12)isep=isep+2
  if(iiu.eq.16)filename(3:6)='p200'
  if(iiu.eq.15)filename(3:6)='p180'
  if(iiu.eq.14)filename(3:6)='p160'
  if(iiu.eq.13)filename(3:6)='p140'
  if(iiu.eq.12)filename(3:6)='p120'
  if(iiu.eq.11)filename(3:6)='p100'
  if(iiu.eq.10)filename(3:6)='p090'
  if(iiu.eq.9)filename(3:6)='p080'
  if(iiu.eq.8)filename(3:6)='p070'
  if(iiu.eq.7)filename(3:6)='p060'
  if(iiu.eq.6)filename(3:6)='p050'
  if(iiu.eq.5)filename(3:6)='p040'
  if(iiu.eq.4)filename(3:6)='p030'
  if(iiu.eq.3)filename(3:6)='p020'
  if(iiu.eq.2)filename(3:6)='p010'
  if(iiu.eq.1)filename(3:6)='p005'
  open(81,file=filename,status='old')
  icou=0
  do 100 i=1,1000
    read(81,*,end=999)adum(i),tdum(i)
100  icou=icou+1
999  if(iiu.lt.11)write(82,110)iiu-1,icou,iiu-1,icou
    if(iiu.eq.11)write(82,111)iiu-1,icou,iiu-1,icou
    if(iiu.gt.11)write(82,111)isep,icou,isep,icou
110  format(6x,'dimension a1',i1,'0(',i3,')',t',i1,'0(',i3,')')
111  format(6x,'dimension a1',i2,'0(',i3,')',t',i2,'0(',i3,')')
    if(iiu.lt.11)write(82,115)iiu-1,icou
    if(iiu.eq.11)write(82,116)iiu-1,icou
    if(iiu.gt.11)write(82,116)isep,icou
115  format(6x,'data n',i1,'0/',i3, '/')
116  format(6x,'data n',i2,'0/',i3, '/')
    do 200 i=1,icou
      if(iiu.lt.11)write(82,120)iiu-1,i,adum(i),iiu-1,i,tdum(i)
      if(iiu.eq.11)write(82,121)iiu-1,i,adum(i),iiu-1,i,tdum(i)
      if(iiu.gt.11)write(82,121)isep,i,adum(i),isep,i,tdum(i)
120  format(6x,'data a1',i1,'0(',i3,')/',i1,e13.7,
1  ' ',t',i1,'0(',i3,')/',i1,e13.7, '/')
121  format(6x,'data a1',i2,'0(',i3,')/',i2,e13.7,
1  ' ',t',i2,'0(',i3,')/',i2,e13.7, '/')
200  continue
    close(81)
90  continue
  stop
end

```

APPENDIX D

SAMPLE OF SUBROUTINE TO BE
INCLUDED INTO A ONE-, TWO-, OR THREE-DIMENSIONAL
HYDRODYNAMIC COMPUTATION TO DETERMINE A NEW BURN FRACTION

```
CDECK USRDFB
      FUNCTION USRDFB(FBRN,TIM,DT,PRS,SMP,NP,I,J,K,IMAX,JMAX,KMAX,
1          SDETIN,PDETIN,PBREF,BUSR,CUSR,DUSR)
C
C *****
C
C *** THIS IS A SAMPLE USER-INPUT FUNCTION FOR THE EVALUATION
C      OF EXPLOSIVE DECOMPOSITION
C
C *** THIS MODULE IS ACCESSED WHENEVER BURN MODEL KBURN=-9 IS CHOSEN
C      FROM INPUT
C
C *** DEFINITION OF INPUT PARAMETERS -
C      USRDFB  OUT   CURRENT VALUE OF BURN RATE
C      FBRN    INP   'OLD' VALUE OF BURN FRACTION
C              OUT   'NEW' VALUE OF BURN FRACTION
C      TIM     INP   CURRENT TIME
C      DT      INP   CURRENT TIME STEP
C      PRS     INP   CURRENT LOCAL PRESSURE
C      SMP     INP   CURRENT LOCAL TEMPERATURE
C      NP      INP   CURRENT EXTERNAL MATERIAL NUMBER
C      I       INP   CELL INDEX  (I-DIRECTION)
C      J       INP   CELL INDEX  (J-DIRECTION)
C      K       INP   CELL INDEX  (K-DIRECTION)
C      IMAX    INP   MAXIMUM NUMBER OF CELLS  (I-DIRECTION)
C      JMAX    INP   MAXIMUM NUMBER OF CELLS  (J-DIRECTION)
C      KMAX    INP   MAXIMUM NUMBER OF CELLS  (K-DIRECTION)
C      SDETIN  INP   USER DEFINED - SUGGESTED: INITIATION TIME
C      PDETIN  INP   USER DEFINED - SUGGESTED: INITIATION PRESSURE
C      PBREF   INP   USER DEFINED - SUGGESTED: REFERENCE PRESSURE
C      BUSR    INP   USER DEFINED - SUGGESTED: NONE
C      CUSR    INP   USER DEFINED - SUGGESTED: NONE
C      DUSR    INP   USER DEFINED - SUGGESTED: NONE
C
C
C
C *** THIS ROUTINE SHOULD RETURN -
C      EITHER  A BURN RATE BY MEANS OF THE FUNCTION NAME
C      OR      AN UPDATED VALUE OF THE BURN FRACTION VIA FBRN
C      THE APPROPRIATE DEFINITION IS DONE DEPENDING ON -
C      IF ON OUTPUT FBRN IS FOUND TO HAVE CHANGED ITS VALUE,
C      THEN THE UPDATED VALUE OF FBRN IS USED
```

```

C      (IN THIS CASE IT IS ADVISABLE TO DEFINE USRDFB=0.)
C      OTHERWISE A BURN RATE DEFINITION IS ASSUMED
C
C      *****
C      IF (PRS.LT.5.E9) RETURN
C      SFB=FBRN
C      ZZFD=0.0
C      IF (FBRN.GE.1.E-5) ZZFD=FBRN
C      CALL BEEN (ZZFD, TIM, DT, PRS, SMP, NP, I, J, K, IMAX, JMAX, KMAX,
1      SDETIN, PDETIN, PBREF, BUSR, CUSR, DUSR)
C      IF (ZZFD.GE.1.E-5) THEN
C      FBRN=ZZFD
C      USRDFB=0.0
C      ELSE
C      FBRN=SFB
C      USRDFB=1.E-20
C      ENDIF
C      RETURN
C      END
C      SUBROUTINE BEEN (FBRN, TIM, DT, PRS, SMP, NP, I, J, K, IMAX, JMAX, KMAX,
1      SDETIN, PDETIN, PBREF, BUSR, CUSR, DUSR)
C      DATA CV/2.09E-5/, AJWL/8.524011/, BJWL/0.1801812/, OMJWL/0.38/
C      DATA R1JWL/4.6/, R2JWL/1.3/, CJWL/0.012066373/
C      DATA TDT/.6666667/, TLIM/1.E-3/
C      INCLUDE 'LAMFILE.FOR'
C      INCLUDE 'HSDATA.FOR'
C      common/icjckc/ IC(1000), JC(1000), KC(1000), FCC(1000)
C      PUT DT INTO MICROSECOND UNITS AND SAVE ORIGINAL VALUE OF DT
C      SAVEDT=DT
C      DT=DT*1.E6
C      IN GENERAL, PCJ SHOULD EQUAL PBREF, THE CJ PRESSURE IN THE INPUT
C      IE PCJ = PBREF/1.E12 TO GET TO MEGABARS.
C      PCJ=PBREF/1.E12
C      PRES IS IN UNITS OF MEGABARS, PRS IN UNITS OF MICROBARS
C      PRES=PRS/1.E12
C      USE 5 KBAR AS MINIMUM PRESSURE FOR REACTION TO OCCUR BASED ON GENERAL
C      PURPOSE PROGRAM RESULTS
C      MINIMUM PRESSURE SHOULD CORRESPOND TO VALUE IN PO(NRS) FROM HS.INFO
C      THE POINT BELOW WHICH THE GENERAL PURPOSE PROGRAM DOES NOT GO
C      IF (PRES.LT.0.00501) THEN
C      DT=SAVEDT
C      RETURN
C      ENDIF
C      IGOTOSUR=0
C      IF (PRES.GT.0.200) IGOTOSUR=1
C      DETERMINE ALAMHS BY LOOKING UP TABLE OF DATA
C      IF FBRN GE AHS USE SURFACE BURN, IF FBRN LT AHS USE NSWC MODEL
C      IREAD=0
C      IPICK=0
C      IF (BUSR.LT.1.E10.AND.FBRN.LT.TLIM.AND.FBRN.GE.0.0) THEN
C      IBUSR=IFIX (BUSR+0.00001)
C      DO 95 KDC=1, IBUSR
C      IF (IC (KDC) .EQ. I .AND. JC (KDC) .EQ. J .AND. KC (KDC) .EQ. K) THEN
C      IPICK=1
C      FBRN=FBRN+FCC (KDC)
C      ENDIF
95      CONTINUE

```

```

IREAD=1
ENDIF
SAVEFBRN=FBRN
IF (IGOTOSUR.EQ.1) GOTO 338
NRSM1=NRS-1
DO 400 ICP=1,NRSM1
  IF (PRES.GE.PO(ICP+1).AND.PRES.LT.PO(ICP)) THEN
    ICP1=ICP+1
    AHS=(ALAMHS(ICP1)-ALAMHS(ICP))*(PRES-PO(ICP))/
1    (PO(ICP1)-PO(ICP))+ALAMHS(ICP)
    THS=(THS(ICP1)-THS(ICP))*(PRES-PO(ICP))/
1    (PO(ICP1)-PO(ICP))+THS(ICP)
    GOTO 401
  ENDIF
400 CONTINUE
401 CONTINUE
  IF (FBRN.LT.AHS.AND.FBRN.GE.0.0) THEN
C  USE NSWC MODEL RELATIONS TO FIND FBRN
    IF (PRES.GE.0.18) THEN
      CALL AFORP(AL180,T180,AL200,T200,N180,N200,FBRN,
1      DT,PRES,PO(21),PO(1),PCJ,THS(21),THS(1),AHS,TAHS)
    ELSEIF (PRES.LT.0.18.AND.PRES.GE.0.16) THEN
      CALL AFORP(AL160,T160,AL180,T180,N160,N180,FBRN,
1      DT,PRES,PO(41),PO(21),PCJ,THS(41),THS(21),AHS,TAHS)
    ELSEIF (PRES.LT.0.16.AND.PRES.GE.0.14) THEN
      CALL AFORP(AL140,T140,AL160,T160,N140,N160,FBRN,
1      DT,PRES,PO(61),PO(41),PCJ,THS(61),THS(41),AHS,TAHS)
    ELSEIF (PRES.LT.0.14.AND.PRES.GE.0.12) THEN
      CALL AFORP(AL120,T120,AL140,T140,N120,N140,FBRN,
1      DT,PRES,PO(81),PO(61),PCJ,THS(81),THS(61),AHS,TAHS)
    ELSEIF (PRES.LT.0.12.AND.PRES.GE.0.1) THEN
      CALL AFORP(AL100,T100,AL120,T120,N100,N120,FBRN,
1      DT,PRES,PO(101),PO(81),PCJ,THS(101),THS(81),AHS,TAHS)
    ELSEIF (PRES.LT.0.1.AND.PRES.GE.0.09) THEN
      CALL AFORP(AL90,T90,AL100,T100,N90,N100,FBRN,
1      DT,PRES,PO(111),PO(101),PCJ,THS(111),THS(101),AHS,TAHS)
    ELSEIF (PRES.LT.0.09.AND.PRES.GE.0.08) THEN
      CALL AFORP(AL80,T80,AL90,T90,N80,N90,FBRN,
1      DT,PRES,PO(121),PO(111),PCJ,THS(121),THS(111),AHS,TAHS)
    ELSEIF (PRES.LT.0.08.AND.PRES.GE.0.07) THEN
      CALL AFORP(AL70,T70,AL80,T80,N70,N80,FBRN,
1      DT,PRES,PO(131),PO(121),PCJ,THS(131),THS(121),AHS,TAHS)
    ELSEIF (PRES.LT.0.07.AND.PRES.GE.0.06) THEN
      CALL AFORP(AL60,T60,AL70,T70,N60,N70,FBRN,
1      DT,PRES,PO(141),PO(131),PCJ,THS(141),THS(131),AHS,TAHS)
    ELSEIF (PRES.LT.0.06.AND.PRES.GE.0.05) THEN
      CALL AFORP(AL50,T50,AL60,T60,N50,N60,FBRN,
1      DT,PRES,PO(151),PO(141),PCJ,THS(151),THS(141),AHS,TAHS)
    ELSEIF (PRES.LT.0.05.AND.PRES.GE.0.04) THEN
      CALL AFORP(AL40,T40,AL50,T50,N40,N50,FBRN,
1      DT,PRES,PO(161),PO(151),PCJ,THS(161),THS(151),AHS,TAHS)
    ELSEIF (PRES.LT.0.04.AND.PRES.GE.0.03) THEN
      CALL AFORP(AL30,T30,AL40,T40,N30,N40,FBRN,
1      DT,PRES,PO(171),PO(161),PCJ,THS(171),THS(161),AHS,TAHS)
    ELSEIF (PRES.LT.0.03.AND.PRES.GE.0.02) THEN
      CALL AFORP(AL20,T20,AL30,T30,N20,N30,FBRN,
1      DT,PRES,PO(181),PO(171),PCJ,THS(181),THS(171),AHS,TAHS)

```

```

ELSEIF (PRES.LT.0.02.AND.PRES.GE.0.01) THEN
CALL AFORP (AL10, T10, AL20, T20, N10, N20, FBRN,
1 DT, PRES, PO (191), PO (181), PCJ, THS (191), THS (181), AHS, TAHS)
ELSEIF (PRES.LT.0.01) THEN
CALL AFORP (AL00, T00, AL10, T10, N00, N10, FBRN,
1 DT, PRES, PO (NRS), PO (191), PCJ, THS (NRS), THS (191), AHS, TAHS)
ENDIF
ENDIF
AFORPFBRN=FBRN
338 CONTINUE
C IF (FBRN.GE.AHS.AND.FBRN.LT.1.0) THEN
IF (FBRN.LT.1.0) THEN
FBRN=SAVEFBRN
C USE SURFACE BURN RELATIONS TO FIND FBRN
CALL SURKIM (PRES, FBRN, DT, AHS)
ENDIF
SURKIMFBRN=FBRN
BRATE1=(AFORPFBRN-SAVEFBRN)/DT
BRATE2=(SURKIMFBRN-SAVEFBRN)/DT
C FBRN IS CURRENTLY FROM SURKIM, CHANGE IF BRATE1 FBRN FROM AFORP IS
LESS
IF (BRATE1.LE.BRATE2) FBRN=AFORPFBRN
DT=SAVEDT
IF (FBRN.GE.TLIM.AND.IREAD.EQ.0) GOTO 774
IF (FBRN.EQ.0.0.AND.IREAD.EQ.0) GOTO 774
IF (FBRN.LT.TLIM.AND.IREAD.EQ.0.AND.FBRN.GT.0.0) THEN
IF (BUSR.LT.1.E10) BUSR=BUSR+1.
IF (BUSR.GT.1.E10) BUSR=1.
IBUSR=IFIX (BUSR+0.00001)
IC (IBUSR)=I
JC (IBUSR)=J
KC (IBUSR)=K
FCC (IBUSR)=FBRN
ELSEIF (FBRN.GE.TLIM.AND.IREAD.EQ.1.AND.IPICK.EQ.1) THEN
IKF=0
DO 96 KDC=1, IBUSR
IF (IKF.EQ.1) IC (KDC-1)=IC (KDC)
IF (IKF.EQ.1) JC (KDC-1)=JC (KDC)
IF (IKF.EQ.1) KC (KDC-1)=KC (KDC)
IF (IKF.EQ.1) FCC (KDC-1)=FCC (KDC)
IF (IC (KDC).EQ.I.AND.JC (KDC).EQ.J.AND.KC (KDC).EQ.K) IKF=1
96 CONTINUE
IBUSR=IBUSR-1
BUSR=BUSR-1.
ELSEIF (FBRN.LT.TLIM.AND.IREAD.EQ.1.AND.IPICK.EQ.1) THEN
DO 97 KDC=1, IBUSR
IF (IC (KDC).EQ.I.AND.JC (KDC).EQ.J.AND.KC (KDC).EQ.K)
1 FCC (KDC)=FBRN
97 CONTINUE
ELSEIF (FBRN.LT.TLIM.AND.IREAD.EQ.1.AND.IPICK.EQ.0) THEN
BUSR=BUSR+1
IBUSR=IFIX (BUSR+0.00001)
IC (IBUSR)=I
JC (IBUSR)=J
KC (IBUSR)=K
FCC (IBUSR)=FBRN
ENDIF

```



```

774  CONTINUE
      RETURN
      END
      SUBROUTINE AFORP (A1,T1,A2,T2,N1,N2,FBRN,DT,PRES,PRES1,PRES2,PCJ,
1      THS1,THS2,AHS,TAHS)
C FBRN:      INPUT -OLD BURN FRACTION
C      OUTPUT -NEW BURN FRACTION
      DIMENSION A1 (N1),T1 (N1),A2 (N2),T2 (N2),AAVE (1000),TAVE (1000)
      INCLUDE 'HSDATA.FOR'
      IF (N1.NE.N2) STOP 123
      QUANX=(PCJ/PRES)**.15
      QUANY=(PCJ/PRES)**.05
      N1M1=N1-1
      DO 100 IR=1,N1
        AAVE (IR)=(A2 (IR)-A1 (IR)) * (PRES-PRES1) / (PRES2-PRES1)+A1 (IR)
        TAVE (IR)=(T2 (IR)-T1 (IR)) * (PRES-PRES1) / (PRES2-PRES1)+T1 (IR)
100    CONTINUE
      IF (FBRN.EQ.0.0) THEN
        TBN=DT
      ELSE
        FBNSCL=ALOG10 ((FBRN/AHS)**QUANY)
C  NEED TO FIND OLD TIME
        DO 110 I=1,N1M1
          IF (AAVE (I).LT.FBNSCL.AND.AAVE (I+1).GE.FBNSCL) THEN
            TBOSCL=(FBNSCL-AAVE (I)) * (TAVE (I+1)-TAVE (I)) /
1            (AAVE (I+1)-AAVE (I))+TAVE (I)
            GOTO 111
          ENDIF
110    CONTINUE
111    CONTINUE
        TBO=TAHS*((10.**TBOSCL)**(1./QUANX))
        TBN=TBO+DT
      ENDIF
      IF (TBN.GT.TAHS) THEN
        FBRN=AHS
        USED=TAHS-TBO
        SDT=DT-USED
        IF (SDT.GT.0.0) DT=SDT
        RETURN
      ELSE
        TBNSCL=ALOG10 ((TBN/TAHS)**QUANX)
        DO 120 I=1,N1M1
          IF (TAVE (I).LT.TBNSCL.AND.TAVE (I+1).GE.TBNSCL) THEN
            FBNSCL=(TBNSCL-TAVE (I)) * (AAVE (I+1)-AAVE (I)) /
1            (TAVE (I+1)-TAVE (I))+AAVE (I)
            GOTO 121
          ENDIF
120    CONTINUE
121    CONTINUE
      ENDIF
      FBRN=AHS*((10.**FBNSCL)**(1./QUANY))
      RETURN
      END
      SUBROUTINE SURKIM(PRES,FBRN,DT,AHS)
      DATA CV/2.09E-5/, AJWL/8.524011/, BJWL/0.1801812/, OMJWL/0.38/
      DATA R1JWL/4.6/, R2JWL/1.3/, CJWL/0.012066373/
      DATA TDT/.6666667/,ALP/1.2/,BET/-0.4/,DEL/32500./,EP/2.5/

```

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```
DATA ROORG/.01/,RIORG/.0039/,ANVAL/0.9/
SBR=3.*.00627/ROORG
DSLAM=SBR*(FBRN**TDT*ALP*PRES** (BET+ANVAL) +
1      (1.-FBRN)**TDT*DEL*PRES** (EP+ANVAL) )
FBRN=FBRN+DT*DSLAM
FBRN=AMIN1 (FBRN,1.)
RETURN
END
```

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